

## SEARCH REQUEST FORM

## Scientific and Technical Information Center

Requester's Full Name: L. G. Gwin Examiner #: 77000 Date: 8/28/00  
 Art Unit: 1713 Phone Number 306-5701 Serial Number: 09/761625  
 Mail Box and Bldg/Room Location: CP3-9A11 Results Format Preferred (circle): PAPER DISK E-MAIL  
CP3-9A11

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover-sheet, pertinent claims, and abstract.

Title of Invention: Stabilization of Polymers after Fixation

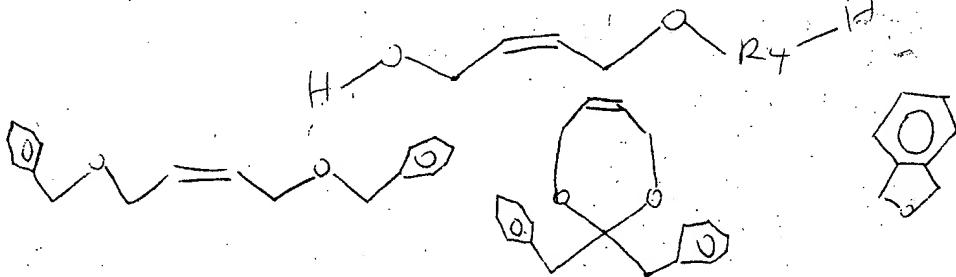
Inventors (please provide full names): Qi Wang

Earliest Priority Filing Date: 3/99

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search for the compound(s) of  
Claim 2 in any type of polymeric  
 composition. Do not limit the search  
 to stabilizers.

Focus on the following:



Thc12

STAFF USE ONLY		Type of Search	Vendors and cost where applicable
Searcher: <u>ED</u>	NA Sequence (#)	STN	<u>\$265.59</u>
Searcher Phone #: _____	AA Sequence (#)	Dialog	_____
Searcher Location: _____	Structure (#)	Questel/OFFP	_____
Date Searcher Picked Up: _____	Bibliographic	and	DB Link
Date Completed: <u>8-28-02</u>	Litigation	Lexis/Nexis	_____
Searcher Prep & Review Time: <u>5</u>	Fulltext	Sequence Systems	_____
Clerical Prep Time: _____	Patent Family	WWW/Internet	_____
Online Time: <u>70</u>	Other	Other (specify)	_____

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FILE 'REGISTRY' ENTERED AT 17:36:24 ON 28 AUG 2002  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE 'LREGISTRY' ENTERED AT 16:31:23 ON 28 AUG 2002  
L1 STR  
FILE 'REGISTRY' ENTERED AT 16:33:26 ON 28 AUG 2002  
L2 1 S L1  
FILE 'LREGISTRY' ENTERED AT 16:33:43 ON 28 AUG 2002  
FILE 'REGISTRY' ENTERED AT 16:48:16 ON 28 AUG 2002  
L3 SCR 1016 OR 997  
L4 SCR 1339 OR 1298  
L5 SCR 1706 OR 1707  
L6 SCR 1992 OR 2016 OR 2021 OR 2026 OR 1929 OR 1918  
L7 13 S L1 AND L3 AND L4 AND L5 NOT L6  
L8 1107 S L1 AND L3 AND L4 AND L5 NOT L6 FUL  
SAV L8 EGW625C/A  
E C18H20O2/MF  
L9 2162 S E3  
L10 11 S L9 AND L8  
L11 232587 S ?BENZYL?/CNS  
L12 3 S L10 AND L11  
E C19H20O2/MF  
L13 1526 S E3  
L14 0 S L13 AND L8  
L15 5149 S OCOC4/ESS  
L16 1674 S OCOC4/ES  
L17 159 S L8 AND (L15 OR L16)  
L18 0 S L17 AND L11  
L19 13 S L17 AND 3/NRS  
E C8H8O/MF  
L20 395 S E3  
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L22 23 S L21  
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L23 57044 S 333.84.17/RID  
L24 2 S L20 AND L23  
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L25 STR

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L27        27 S L25 SSS FUL SUB=L8

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FILE 'HCA' ENTERED AT 17:23:10 ON 28 AUG 2002

L28        1214958 S STABL? OR STABIL?

L29        593319 S POLYVINYL##(2A)CHLORIDE# OR POLY(2A)VINYL##(2A)CHLORIDE

L30        36 S L12

L31        146 S L24

L32        165 S L27

L33        3 S L30 AND L28

L34        2 S L30 AND L29

L35        3 S L33 OR L34

L36        12 S L31 AND L28

L37        4 S L31 AND L29

L38        13 S L36 OR L37

L39        7 S L32 AND L28

L40        2 S L32 AND L29

L41        7 S L39 OR L40

FILE 'REGISTRY' ENTERED AT 17:26:00 ON 28 AUG 2002

            E POLYVINYL CHLORIDE/CN

L42        1 S E3

            E POLYETHYLENE/CN

L43        1 S E3

            E POLYPROPYLENE/CN

L44        1 S E3

FILE 'HCA' ENTERED AT 17:26:49 ON 28 AUG 2002

L45        251013 S L42 OR L43 OR L44

L46        2 S L30 AND L45

L47        3 S L31 AND L45

L48        2 S L32 AND L45

L49        3 S L35 OR L46

L50        13 S L38 OR L47

L51        7 S L41 OR L48

FILE 'REGISTRY' ENTERED AT 17:36:24 ON 28 AUG 2002

=> d 127 que stat

L1            STR

O×CH2×CH×CH×CH2×O

1    2    3    4    5    6

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE

L3 SCR 1016 OR 997  
L4 SCR 1339 OR 1298  
L5 SCR 1706 OR 1707  
L6 SCR 1992 OR 2016 OR 2021 OR 2026 OR 1929 OR 1918  
L8 1107 SEA FILE=REGISTRY SSS FUL L1 AND L3 AND L4 AND L5 NOT L6  
L25 STR



VAR G1=10/13/17

REP G2=(1-8) 20

NODE ATTRIBUTES:

NSPEC IS RC AT 20  
CONNECT IS E1 RC AT 10  
CONNECT IS E2 RC AT 13  
DEFAULT MLEVEL IS ATOM  
GGCAT IS SAT AT 10  
GGCAT IS SAT AT 13  
GGCAT IS UNS AT 14  
DEFAULT ECLEVEL IS LIMITED  
ECOUNT IS M1-X6 C AT 10

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L27 27 SEA FILE=REGISTRY SUB=L8 SSS FUL L25

100.0% PROCESSED 832 ITERATIONS  
SEARCH TIME: 00.00.03

27 ANSWERS

=> file hca  
FILE 'HCA' ENTERED AT 17:36:58 ON 28 AUG 2002  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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=> d 149 1-3 cbib abs hitstr hitind

L49 ANSWER 1 OF 3 HCA COPYRIGHT 2002 ACS

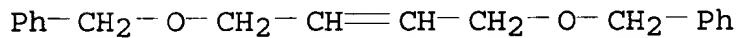
136:247398 Etherification method for producing benzyl ether derivatives of 2-butene-1,4-diols. Krishnamurti, Ramesh; Wang, Qi; Smolka, Thomas F. (Occidental Chemical Corporation, USA; Stephens, Dinah, H.). PCT Int. Appl. WO 2002022537 A2 20020321, 19 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-GB4036 20010910. PRIORITY: US 2000-PV231790 20000911.

AB A method for producing benzyl ethers of 2-butene-1,4-diols, useful as polymer **stabilizers** (no data), comprises reacting 2-butene-1,4-diols (e.g., 2-butene-1,4-diol) with benzyl chlorides (e.g., benzyl chloride) in the presence of an alkali (e.g., sodium hydroxide) or alk. earth metal hydroxide or carbonate, optionally in the presence of a phase-transfer catalyst (e.g., benzyltriethylammonium chloride) to produce mono- and/or di-benzyl ethers of 2-butene-1,4-diols [e.g., 1,4-bis(benzylxy)-2-butene] and recovering at least a portion of at least one such benzene deriv.

IT 70677-94-0P, 1,4-Bis(benzylxy)-2-butene  
(etherification method for producing benzyl ether derivs. of 2-butene-1,4-diols)

RN 70677-94-0 HCA

CN Benzene, 1,1'-[2-butene-1,4-diylbis(oxymethylene)]bis- (9CI) (CA INDEX NAME)



IC ICM C07C041-00

CC 25-9 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 37, 45

IT 70677-94-0P, 1,4-Bis(benzylxy)-2-butene 80885-30-9P  
(etherification method for producing benzyl ether derivs. of 2-butene-1,4-diols)

L49 ANSWER 2 OF 3 HCA COPYRIGHT 2002 ACS

135:93426 **Stabilization** of polymers after exposure to oxidation and article manufacture. Wang, Qi (USA). U.S. Pat. Appl. Publ. US 20010007884 A1 20010712, 9 pp., Cont.-in-part of U. S. Ser. No. 272,843. (English). CODEN: USXXCO. APPLICATION: US 2001-761625 20010117. PRIORITY: US 1999-272843 19990319.

AB **Polyvinyl chloride**, **polyvinylidene chloride**, **polycarbonate**, **polyethylene**, **polypropylene**, **polyamide**, **polyimide**, **polyether**, **polyester**, or **polyvinyl acetate** contg. apprx.0.005-10 phr **stabilizer** are resistant to discoloring after exposure to oxidn. **PVC** contg. 1.34 g **stabilizer** phthalan had initial yellowness

value 17.5, after .gamma. radiation 31.9, and after aging 49.5, vs. 18.1, 50.2, and 75.5, resp., for a control without **stabilizer**.

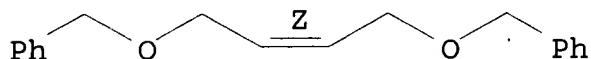
IT 68972-96-3

(**stabilization** of polymers after exposure to oxidn.)

RN 68972-96-3 HCA

CN Benzene, 1,1'-(2Z)-2-butene-1,4-diylbis(oxymethylene)bis- (9CI)  
(CA INDEX NAME)

Double bond geometry as shown.



IT 9002-86-2, Poly(vinyl chloride)

) 9002-88-4, Polyethylene 9003-07-0,  
**Polypropylene**

(**stabilization** of polymers after exposure to oxidn.)

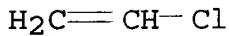
RN 9002-86-2 HCA

CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4

CMF C2 H3 Cl



RN 9002-88-4 HCA

CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 74-85-1

CMF C2 H4



RN 9003-07-0 HCA

CN 1-Propene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 115-07-1

CMF C3 H6

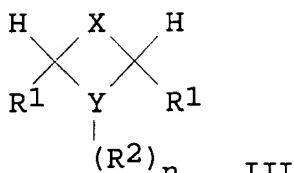
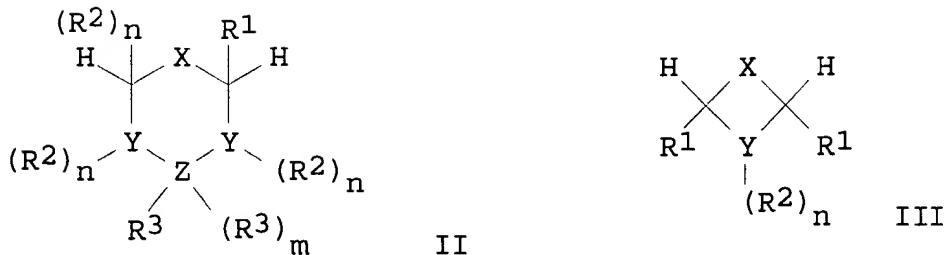
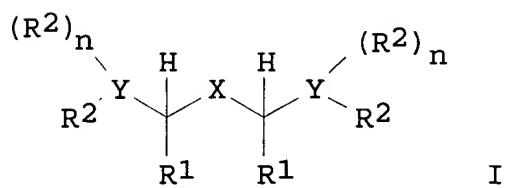


IC ICM C08K005-06  
 ICS C08K005-46  
 NCL 524083000  
 CC 37-6 (Plastics Manufacture and Processing)  
 ST discoloration prevention agents polymer; **PVC** phthalan  
**stabilizer**; polyvinylidene chloride yellowing prevention;  
**polycarbonate** yellowing prevention; **Polyethylene**  
 yellowing prevention; **Polypropylene** yellowing prevention;  
 polyamide yellowing prevention; polyimide yellowing prevention;  
 polyether yellowing prevention; polyester yellowing prevention;  
 polyvinyl acetate yellowing prevention  
 IT Antioxidants  
 Discoloration prevention agents  
 Yellowing prevention  
 (**stabilization** of polymers after exposure to oxidn.)  
 IT Polyamides, uses  
**Polycarbonates**, uses  
 Polyesters, uses  
 Polyethers, uses  
 Polyimides, uses  
**Polyurethanes**, uses  
 (**stabilization** of polymers after exposure to oxidn.)  
 IT 110-65-6, 2-Butyne-1,4-diol 332-77-4 496-14-0, Phthalan  
 589-29-7, 1,4-Benzenedimethanol 1606-85-5, 1,4-Bis(2-hydroxy  
 ethoxy)-2-butyne 2568-24-3 5417-32-3 10192-64-0 21285-46-1  
 67461-24-9 **68972-96-3** 81028-03-7  
 (**stabilization** of polymers after exposure to oxidn.)  
 IT 9002-85-1, Poly(vinylidene chloride) **9002-86-2**,  
**Poly(vinyl chloride)** **9002-88-4**  
 , **Polyethylene** **9003-07-0**, **Polypropylene**  
 9003-20-7, Poly(vinyl acetate)  
 (**stabilization** of polymers after exposure to oxidn.)

L49 ANSWER 3 OF 3 HCA COPYRIGHT 2002 ACS

133:267624 **Stabilization** and discoloration prevention of  
 polymers after exposure to oxidation and antioxidants therefor.  
 Wang, Qi (Occidental Chemical Corporation, USA; Stephens, Dinah).  
 PCT Int. Appl. WO 2000056812 A1 20000928, 37 pp. DESIGNATED STATES:  
 W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,  
 CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN,  
 IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG,  
 MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,  
 TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD,  
 RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES,  
 FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD,  
 TG. (English). CODEN: PIIXD2. APPLICATION: WO 2000-GB247  
 20000128. PRIORITY: US 1999-272843 19990319.

GI



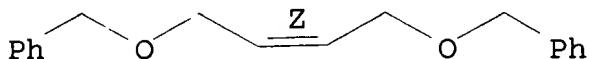
AB **Poly(vinyl chloride), poly(vinylidene chloride), polycarbonates, polyethylene, polypropylene, polyamides, polyimides, polyethers, polyesters, or poly(vinyl acetate) contg. apprx. 0.005-10 phr of a stabilizer I, II, or III, where Z is C, P, Sn, Si, or B; X is -R1C:CR1-, ethynyl, (un)substituted benzene, pyridine, pyrimidine, triazine, furan, pyrrole, thiophene, or naphthalene ring; each Y is independently O, S, or N; each R is independently H, C1-24-alkyl, C6-24-aryl, C7-24-aralkyl; each R1 is independently R, OR, RCO, ROCO, ROCO2, PR2, P(OR)2, PR(OR), NR2, R2NCO, R2NCO2, SR, halogen, or two R1 groups can form a ring; each R2 is independently R, RCO, ROCO, P(OR)2, Sn(R)q(OR)3-q, SnRq(OCOR)3-q, Si(R)q(OR)3-q, BRq(OR)2-q, or two R2 groups can form a ring; each R3 is independently R, RCO, ROCO, ROCO2, OR, SR, NR2, OPR2, or OP(OR)2; m is 0 when Z is P or B and 1 when Z is Sn, Si, or C; n is 0 when Y is O or S and 1 when Y is N; p is 0-4; and q is 0-3 for the tin stabilizers and 0-2 for the boron stabilizers, with the proviso that in I, when X = -CH:CH-, Y = O and R2 = H, at least one of the R1 is not H; and in II, when X = -R1C:CR1-, Y = O and Z = C, then at least one of the R3 groups on Z is not H. Thus, a plaque from a compn. comprising PVC 150.00, stearic acid 0.30, Mark 152S 0.23, dioctyl phthalate 97.50, Drapex 6.8 15.00, and phthalan 1.34 g was irradiated with 50 kGy gamma-rays, and aged 48 h at 50.degree., giving yellowness 17.5 initially, 31.9 after radiation, and 49.5 after aging, compared with 18.1, 50.2, and 75.5, resp., without phthalan.**

IT **68972-96-3, cis-1,4-Bisbenzyloxy-2-butene 70677-94-0 (stabilization and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)**

RN **68972-96-3 HCA**

CN **Benzene, 1,1'-(2Z)-2-butene-1,4-diylbis(oxymethylene)]bis- (9CI) (CA INDEX NAME)**

Double bond geometry as shown.



RN 70677-94-0 HCA  
 CN Benzene, 1,1'-[2-butene-1,4-diylbis(oxymethylene)]bis- (9CI) (CA INDEX NAME)

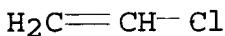


IT 9002-86-2, PVC 9002-88-4,  
 Polyethylene 9003-07-0, Polypropylene  
 (stabilization and discoloration prevention of polymers  
 after exposure to oxidn. and antioxidants therefor)

RN 9002-86-2 HCA  
 CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

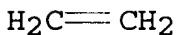
CRN 75-01-4  
 CMF C2 H3 Cl



RN 9002-88-4 HCA  
 CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

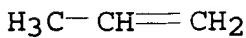
CRN 74-85-1  
 CMF C2 H4



RN 9003-07-0 HCA  
 CN 1-Propene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 115-07-1  
 CMF C3 H6



IC ICM C08K005-00

CC ICS C08K005-053; C08K005-15; C08K005-06  
 37-6 (Plastics Manufacture and Processing)  
 ST antioxidant yellowing prevention polymer; **PVC** phthalan  
 antioxidant gamma radiation; polyolefin antioxidant yellowing  
 prevention; vinyl compd polymer antioxidant yellowing prevention;  
 polycarbonate antioxidant yellowing prevention;  
 polyurethane antioxidant yellowing prevention; polyamide  
 antioxidant yellowing prevention; polyimide antioxidant yellowing  
 prevention; polyether antioxidant yellowing prevention; polyester  
 antioxidant yellowing prevention

IT Yellowing prevention  
 Yellowing prevention  
 (agents; **stabilization** and discoloration prevention of  
 polymers after exposure to oxidn. and antioxidants therefor)

IT Antioxidants  
 (**stabilization** and discoloration prevention of polymers  
 after exposure to oxidn. and antioxidants therefor)

IT Polyamides, uses  
**Polycarbonates**, uses  
 Polyesters, uses  
 Polyethers, uses  
 Polyimides, uses  
**Polyurethanes**, uses  
 (**stabilization** and discoloration prevention of polymers  
 after exposure to oxidn. and antioxidants therefor)

IT Discoloration prevention agents  
 Discoloration prevention agents  
 (yellowing; **stabilization** and discoloration prevention  
 of polymers after exposure to oxidn. and antioxidants therefor)

IT 110-64-5, 2-Butene-1,4-diol 110-65-6, 2-Butyne-1,4-diol  
 332-77-4, 2,5-Dimethoxy-2,5-dihydrofuran 496-14-0, Phthalan  
 589-29-7, 1,4-Benzenedimethanol 1606-85-5, 1,4-Bis(2-  
 hydroxyethoxy)-2-butyne 2568-24-3, 4,7-Dihydro-2-phenyl-1,3-  
 dioxepin 10192-64-0 21285-46-1 67461-24-9 **68972-96-3**  
 , cis-1,4-Bisbenzyloxy-2-butene **70677-94-0** 81028-03-7,  
 cis-4-Benzyloxy-2-buten-1-ol  
 (**stabilization** and discoloration prevention of polymers  
 after exposure to oxidn. and antioxidants therefor)

IT 9002-85-1, Poly(vinylidene chloride) **9002-86-2**,  
**PVC** **9002-88-4**, **Polyethylene**  
 9003-07-0, **Polypropylene** 9003-20-7, Poly(vinyl  
 acetate)  
 (**stabilization** and discoloration prevention of polymers  
 after exposure to oxidn. and antioxidants therefor)

=> d 150 1-13 cbib abs hitstr hitind

L50 ANSWER 1 OF 13 HCA COPYRIGHT 2002 ACS

137:78570 Conformational **stabilization** of phthalan: physical  
 origin of tiny ring-puckering barrier. Jeon, Sangmi; Choo, Jaebum;  
 Kim, Sungwhan; Kwon, Younghui; Kim, Jin-Yeol; Lee, Young-Il; Chung,

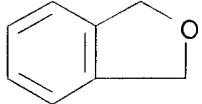
Hoeil (Department of Chemistry, Hanyang University, Ansan, 425-791, S. Korea). Journal of Molecular Structure, 609(1-3), 159-167 (English) 2002. CODEN: JMSB4. ISSN: 0022-2860. Publisher: Elsevier Science B.V..

AB The conformational property of phthalan has been investigated using ab initio calcn. and natural bond orbital (NBO) anal. methods. Geometry optimizations for the planar (C<sub>2</sub>v) and puckered (Cs) conformers have been carried out using the HF, B3LYP, and MP methods, and the results indicate that this mol. has a tiny ring-puckering barrier. This barrier appears to be in good agreement with the previous exptl. result. NBO anal. shows that the tiny ring-puckering barrier is closely related to the MO interactions around the C-O bonds of the five-membered ring. The gas-phase IR and liq.-phase Raman spectra of phthalan and 1,3-benzodioxole have been recorded and analyzed in terms of C<sub>2</sub>v symmetry. Vibrational frequency calcns. using the B3LYP method have also been performed to compare with the spectroscopic data. The B3LYP frequency calcns. do a reasonable job of estg. the frequencies.

IT 496-14-0, Phthalan  
(ab initio and NBO study on conformational **stabilization** of phthalan)

RN 496-14-0 HCA

CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 22-3 (Physical Organic Chemistry)  
Section cross-reference(s): 73

ST phthalan conformational **stabilization** ab initio NBO

IT Density functional theory  
(B3LYP; ab initio and NBO study on conformational **stabilization** of phthalan)

IT Ab initio methods  
Basis sets  
Conformation  
Conformational barrier  
Conformational potential  
Conformers  
Electron correlation  
Electron delocalization  
HF MO (molecular orbital)  
Hyperconjugation  
MP2 (Moller-Plesset)  
MP3 (Moller-Plesset)  
MP4 (Moller-Plesset)  
Molecular vibration  
Natural bond orbital

Normal modes  
 QCISD(T) (molecular orbital)  
 Total energy  
 Vibrational frequency  
 (ab initio and NBO study on conformational **stabilization**  
 of phthalan)

IT IR spectra  
 Raman spectra  
 (exptl. and calcd.; ab initio and NBO study on conformational  
**stabilization** of phthalan)

IT IR spectra  
 (far-IR; ab initio and NBO study on conformational  
**stabilization** of phthalan)

IT IR spectra  
 (mid-IR; ab initio and NBO study on conformational  
**stabilization** of phthalan)

IT Molecular structure  
 (optimized; ab initio and NBO study on conformational  
**stabilization** of phthalan)

IT Molecular vibration  
 (puckering, ring puckering; ab initio and NBO study on  
 conformational **stabilization** of phthalan)

IT Potential barrier  
 (ring-puckering; ab initio and NBO study on conformational  
**stabilization** of phthalan)

IT 496-11-7, Indan 496-14-0, Phthalan  
 (ab initio and NBO study on conformational **stabilization**  
 of phthalan)

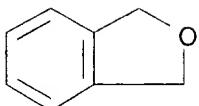
IT 274-09-9, 1,3-Benzodioxole  
 (ab initio and NBO study on conformational **stabilization**  
 of phthalan)

L50 ANSWER 2 OF 13 HCA COPYRIGHT 2002 ACS  
 135:332065 Thermoplastic resin composition. Kanayama, Satoshi;  
 Hatakeyama, Tatsuhiko; Miya, Shinya; Narita, Kenichi; Honma, Ken  
 (Japan). U.S. Pat. Appl. Publ. US 20010034419 A1 20011025, 20 pp.,  
 Cont.-in-part of WO1999JP 9904007. (English). CODEN: USXXCO.  
 APPLICATION: US 2001-768931 20010124. PRIORITY: JP 1998-212461  
 19980728; WO 1999-JP4007 19990727; JP 2000-15530 20000125; JP  
 2000-15531 20000125; JP 2000-15889 20000125; JP 2000-16033 20000125.

AB A thermoplastic resin compn. comprising: a transparent arom.  
 thermoplastic resin (a) and a copolyester resin (b) comprising at  
 least two kinds of dicarboxylic acid moieties and one kind of diol  
 moiety, 1 to 50 mol of the dicarboxylic acid moieties being a  
 naphthalenedicarboxylic acid moiety, the ratio of (a) to the  
 combined amt. of (a) and (b) being 55-99.99 by wt., and the ratio of  
 (b) being 0.01-45 by wt.

IT 496-14-0  
 (ionizing radiation **stabilizer**; thermoplastic resin  
 compn.)

RN 496-14-0 HCA  
 CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)

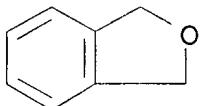


IC C08F020-00  
 NCL 525439000  
 CC 37-3 (Plastics Manufacture and Processing)  
 Section cross-reference(s): 63  
 IT Polyoxoalkylenes, uses  
     /ionizing radiation **stabilizer**; thermoplastic resin  
     compn.)  
 IT Polycarbonates, uses  
     Polyesters, uses  
     (thermoplastic resin compn.)  
 IT 80-48-8, Methyl p-toluene sulfonate 100-51-6, Benzyl alcohol, uses  
     101-49-5, 2-Benzyl-1,3-dioxolane 102-04-5, Dibenzyl ketone  
     103-41-3, Benzyl cinnamate 103-50-4, Dibenzyl ether 103-54-8,  
     Cinnamyl acetate 104-54-1, Cinnamyl alcohol 110-88-3, Trioxane,  
     uses 119-53-9, Benzoin 119-61-9, Benzophenone, uses 120-51-4,  
     Benzyl benzoate 122-69-0, Cinnamyl cinnamate 123-63-7,  
     Paraldehyde 300-57-2, Allylbenzene 462-95-3, Diethoxy methane  
     496-14-0 538-74-9, Dibenzylsulfide 574-09-4, Benzoin  
     ethyl ether 620-32-6, Dibenzyl sulfone 621-08-9, Dibenzyl  
     sulfoxide 622-22-0, 1,2-Dibenzylxyloxy ethane 640-60-8, Phenyl  
     p-toluenesulfonate 649-15-0 696-59-3, 2,5-Dimethoxy  
     tetrahydrofuran 772-00-9, 4-Phenyl-1,3-dioxane 945-51-7,  
     Diphenyl sulfoxide 947-19-3, 1-Hydroxy cyclohexyl phenyl ketone  
     1696-20-4 1746-13-0, Allyl phenyl ether 2550-40-5, Dicyclohexyl  
     disulfide 2568-25-4, 4-Methyl-2-phenyl-1,3-dioxolane 6175-45-7,  
     2,2-Diethoxy acetophenone 6543-04-0, 2,2'-Trimethylenebis1,3-  
     dioxolane 6770-38-3, 1,4-Bis-methoxymethyl benzene 9006-24-0,  
     NIKANOL Y-50 17178-10-8 25322-69-4, Uniol D-2000 26403-62-3,  
     Unisafe NKL-9520 56262-45-4, IUPILON FR-53 91528-47-1, Ethyl  
     dimethyl aminobenzoate 151183-90-3, NIKANOL DS  
     /ionizing radiation **stabilizer**; thermoplastic resin  
     compn.)

L50 ANSWER 3 OF 13 HCA COPYRIGHT 2002 ACS  
 135:93426 **Stabilization** of polymers after exposure to  
     oxidation and article manufacture. Wang, Qi (USA). U.S. Pat. Appl.  
     Publ. US 20010007884 A1 20010712, 9 pp., Cont.-in-part of U. S. Ser.  
     No. 272,843. (English). CODEN: USXXCO. APPLICATION: US  
     2001-761625 20010117. PRIORITY: US 1999-272843 19990319.  
 AB **Polyvinyl chloride**, polyvinylidene  
     chloride, **polycarbonate**, **polyethylene**,  
     **polypropylene**, polyamide, polyimide, polyether, polyester,  
     or polyvinyl acetate contg. .aprx.0.005-10 phr **stabilizer**  
     are resistant to discoloring after exposure to oxidn. PVC  
     contg. 1.34 g **stabilizer** phthalan had initial yellowness

value 17.5, after .gamma. radiation 31.9, and after aging 49.5, vs. 18.1, 50.2, and 75.5, resp., for a control without **stabilizer**.

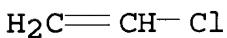
IT 496-14-0, Phthalan  
(**stabilization** of polymers after exposure to oxidn.)  
RN 496-14-0 HCA  
CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



IT 9002-86-2, Poly(vinyl chloride)  
) 9002-88-4, Polyethylene 9003-07-0,  
**Polypropylene**  
(**stabilization** of polymers after exposure to oxidn.)  
RN 9002-86-2 HCA  
CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

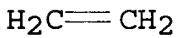
CRN 75-01-4  
CMF C2 H3 Cl



RN 9002-88-4 HCA  
CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

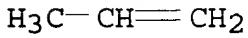
CRN 74-85-1  
CMF C2 H4



RN 9003-07-0 HCA  
CN 1-Propene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 115-07-1  
CMF C3 H6

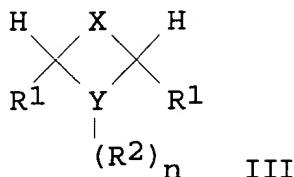
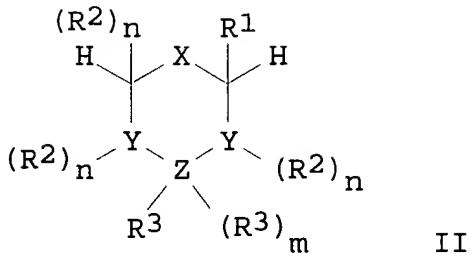
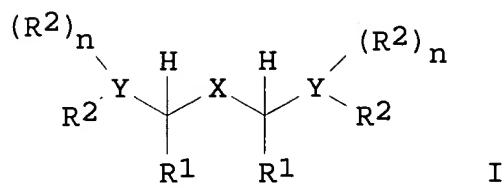


IC ICM C08K005-06

NCL ICS C08K005-46  
 524083000  
 CC 37-6 (Plastics Manufacture and Processing)  
 ST discoloration prevention agents polymer; **PVC** phthalan  
**stabilizer**; polyvinylidene chloride yellowing prevention;  
**polycarbonate** yellowing prevention; **Polyethylene**  
 yellowing prevention; **Polypropylene** yellowing prevention;  
 polyamide yellowing prevention; polyimide yellowing prevention;  
 polyether yellowing prevention; polyester yellowing prevention;  
 polyvinyl acetate yellowing prevention  
 IT Antioxidants  
 Discoloration prevention agents  
 Yellowing prevention  
 (**stabilization** of polymers after exposure to oxidn.)  
 IT Polyamides, uses  
**Polycarbonates**, uses  
 Polyesters, uses  
 Polyethers, uses  
 Polyimides, uses  
**Polyurethanes**, uses  
 (**stabilization** of polymers after exposure to oxidn.)  
 IT 110-65-6, 2-Butyne-1,4-diol 332-77-4 **496-14-0**, Phthalan  
 589-29-7, 1,4-Benzenedimethanol 1606-85-5, 1,4-Bis(2-hydroxy  
 ethoxy)-2-butyne 2568-24-3 5417-32-3 10192-64-0 21285-46-1  
 67461-24-9 68972-96-3 81028-03-7  
 (**stabilization** of polymers after exposure to oxidn.)  
 IT 9002-85-1, Poly(vinylidene chloride) **9002-86-2**,  
**Poly(vinyl chloride)** **9002-88-4**  
 , **Polyethylene** **9003-07-0**, **Polypropylene**  
 9003-20-7, Poly(vinyl acetate)  
 (**stabilization** of polymers after exposure to oxidn.)

L50 ANSWER 4 OF 13 HCA COPYRIGHT 2002 ACS  
 134:326142 Thermal Reactions of Isodihydrobenzofuran: Experimental  
 Results and Computer Modeling. Lifshitz, Assa; Suslensky, Aya;  
 Tamburu, Carmen (Department of Physical Chemistry, The Hebrew  
 University of Jerusalem, Jerusalem, 91904, Israel). Journal of  
 Physical Chemistry A, 105(13), 3148-3157 (English) 2001. CODEN:  
 JPCAFH. ISSN: 1089-5639. Publisher: American Chemical Society.  
 AB The thermal reactions of isodihydrobenzofuran (phthalan) were  
 studied behind reflected shock waves in a single pulse shock tube  
 over the temp. range 1050-1300 K and overall densities of .aprx.3  
 .times. 10<sup>-5</sup> mol/cm<sup>3</sup>. The total decompr. rate, expressed as a  
 first-order rate const., is 1012.10 exp(-53.7 .times. 103/RT) s<sup>-1</sup>,  
 where R is in given units of cal/(K mol). One isomerization  
 product, o-tolualdehyde [kisomerization] = 1016.50 exp (-80.5  
 .times. 103/RT) s<sup>-1</sup>, and products resulting from unimol. cleavage  
 of the furan ring were obtained under shock heating. Carbon  
 monoxide and toluene are the products of the highest concn.  
 Isobenzofuran is obtained by a 1,6-H<sub>2</sub> elimination from the furan  
 ring with a rate const. k = 1013.78 exp(-70.0 .times. 103/RT) s<sup>-1</sup>.  
 In addn., benzene, ethylbenzene, styrene, ethylene, methane, and



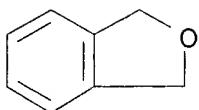


AB **Poly(vinyl chloride), poly(vinylidene chloride), polycarbonates, polyethylene, polypropylene, polyamides, polyimides, polyethers, polyesters, or poly(vinyl acetate) contg. apprx. 0.005-10 phr of a stabilizer I, II, or III, where Z is C, P, Sn, Si, or B; X is -R1C:CR1-, ethynyl, (un)substituted benzene, pyridine, pyrimidine, triazine, furan, pyrrole, thiophene, or naphthalene ring; each Y is independently O, S, or N; each R is independently H, C1-24-alkyl, C6-24-aryl, C7-24-aralkyl; each R1 is independently R, OR, RCO, ROCO, ROCO2, PR2, P(OR)2, PR(OR), NR2, R2NCO, R2NCO2, SR, halogen, or two R1 groups can form a ring; each R2 is independently R, RCO, ROCO, P(OR)2, Sn(R)q(OR)3-q, SnRq(OCOR)3-q, Si(R)q(OR)3-q, BRq(OR)2-q, or two R2 groups can form a ring; each R3 is independently R, RCO, ROCO, ROCO2, OR, SR, NR2, OPR2, or OP(OR)2; m is 0 when Z is P or B and 1 when Z is Sn, Si, or C; n is 0 when Y is O or S and 1 when Y is N; p is 0-4; and q is 0-3 for the tin stabilizers and 0-2 for the boron stabilizers, with the proviso that in I, when X = -CH:CH-, Y = O and R2 = H, at least one of the R1 is not H; and in II, when X = -R1C:CR1-, Y = O and Z = C, then at least one of the R3 groups on Z is not H. Thus, a plaque from a compn. comprising PVC 150.00, stearic acid 0.30, Mark 152S 0.23, dioctyl phthalate 97.50, Drapex 6.8 15.00, and phthalan 1.34 g was irradiated with 50 kGy gamma-rays, and aged 48 h at 50.degree., giving yellowness 17.5 initially, 31.9 after radiation, and 49.5 after aging, compared with 18.1, 50.2, and 75.5, resp., without phthalan.**

IT **496-14-0, Phthalan (stabilization and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)**

RN **496-14-0 HCA**

CN **Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)**



IT 9002-86-2, PVC 9002-88-4,  
 Polyethylene 9003-07-0, Polypropylene  
 (stabilization and discoloration prevention of polymers  
 after exposure to oxidn. and antioxidants therefor)

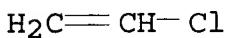
RN 9002-86-2 HCA

CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4

CMF C2 H3 Cl



RN 9002-88-4 HCA

CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 74-85-1

CMF C2 H4



RN 9003-07-0 HCA

CN 1-Propene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 115-07-1

CMF C3 H6



IC ICM C08K005-00

ICS C08K005-053; C08K005-15; C08K005-06

CC 37-6 (Plastics Manufacture and Processing)

ST antioxidant yellowing prevention polymer; PVC phthalan  
 antioxidant gamma radiation; polyolefin antioxidant yellowing  
 prevention; vinyl compd polymer antioxidant yellowing prevention;  
 polycarbonate antioxidant yellowing prevention;  
 polyurethane antioxidant yellowing prevention; polyamide  
 antioxidant yellowing prevention; polyimide antioxidant yellowing

IT prevention; polyether antioxidant yellowing prevention; polyester antioxidant yellowing prevention

IT Yellowing prevention

IT Yellowing prevention  
(agents; **stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT Antioxidants  
(**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT Polyamides, uses

IT Polycarbonates, uses

IT Polyesters, uses

IT Polyethers, uses

IT Polyimides, uses

IT Polyurethanes, uses  
(**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT Discoloration prevention agents

IT Discoloration prevention agents  
(yellowing; **stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT 110-64-5, 2-Butene-1,4-diol 110-65-6, 2-Butyne-1,4-diol  
332-77-4, 2,5-Dimethoxy-2,5-dihydrofuran 496-14-0,  
Phthalan 589-29-7, 1,4-Benzenedimethanol 1606-85-5,  
1,4-Bis(2-hydroxyethoxy)-2-butyne 2568-24-3, 4,7-Dihydro-2-phenyl-  
1,3-dioxepin 10192-64-0 21285-46-1 67461-24-9 68972-96-3,  
cis-1,4-Bisbenzyloxy-2-butene 70677-94-0 81028-03-7,  
cis-4-Benzyloxy-2-buten-1-ol  
(**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT 9002-85-1, Poly(vinylidene chloride) 9002-86-2,  
PVC 9002-88-4, Polyethylene  
9003-07-0, Polypropylene 9003-20-7, Poly(vinyl acetate)  
(**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

L50 ANSWER 6 OF 13 HCA COPYRIGHT 2002 ACS

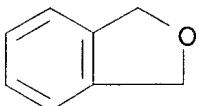
132:63957 Experimental determination of the antiaromaticity of cyclobutadiene. Deniz, Ashok A.; Peters, Kevin S.; Snyder, Gary J. (Dep. Chem., Univ. Chicago, Chicago, IL, 60637, USA). Science (Washington, D. C.), 286(5442), 1119-1122 (English) 1999. CODEN: SCIEAS. ISSN: 0036-8075. Publisher: American Association for the Advancement of Science.

AB Photoacoustic calorimetry was used to quantify the antiaromaticity of 1,3-cyclobutadiene (CBD) by measuring the heat release accompanying its formation via photofragmentation of a polycyclic precursor. In combination with quantum yield measurements and thermochem. calcns., this measurement provides an enthalpy of formation for CBD of 114 .+- . 11 (2.sigma.) kilocalories per mol (kcal/mol). The extraordinary reactivity of this prototypical antiarom. hydrocarbon had previously made its heat of formation

inaccessible except by theor. calcns. Relative to a hypothetical strainless, conjugated diene ref., CBD is destabilized by a total of 87 kcal/mol, 32 kcal/mol of which can be attributed to ring strain and 55 kcal/mol to antiaromaticity (compared with 21 kcal/mol for the arom. **stabilization** of benzene). Relative to a ref. with isolated double bonds, CBD's antiaromaticity is 48 kcal/mol (compared with 32 kcal/mol for the aromaticity of benzene).

IT 496-14-0, Phthalan  
(formation heat; exptl. detn. of antiaromaticity of cyclobutadiene)

RN 496-14-0 HCA  
CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 22-13 (Physical Organic Chemistry)  
IT **Stabilization** energy

(isodesmic, homodesmic and; exptl. detn. of antiaromaticity of cyclobutadiene)

IT 496-14-0, Phthalan  
(formation heat; exptl. detn. of antiaromaticity of cyclobutadiene)

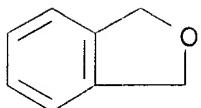
L50 ANSWER 7 OF 13 HCA COPYRIGHT 2002 ACS

125:142504 Electron-Transfer-Induced Reductive Cleavage of Phthalans: Reactivity and Synthetic Applications. Azzena, Ugo; Demartis, Salvatore; Melloni, Giovanni (Dipartimento di Chimica, Universita di Sassari, Sassari, I-07100, Italy). Journal of Organic Chemistry, 61(15), 4913-4919 (English) 1996. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

AB The behavior of phthalan (1,3-dihydroisobenzofuran) was investigated under conditions of electron transfer from alkali metals in aprotic solvents. Reaction with lithium in the presence of a catalytic amt. of naphthalene in THF led to the reductive cleavage of an arylmethyl carbon-oxygen bond, with formation of a **stable** dilithium compd. Trapping of this intermediate with several electrophiles (alkyl halides, carbonyl derivs., CO<sub>2</sub>) was successful. The extension of this procedure to several substituted phthalans was investigated, and the regiochem. as well as the synthetic usefulness of these reactions are discussed.

IT 496-14-0, Phthalan  
(electron-transfer-induced reductive cleavage of phthalan derivs.)

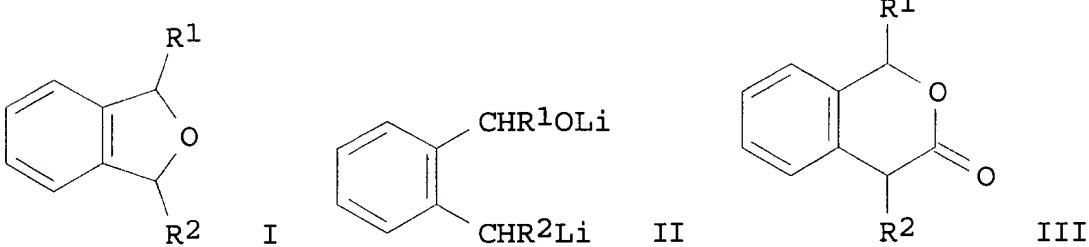
RN 496-14-0 HCA  
CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



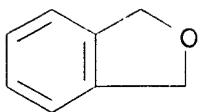
CC 27-14 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 22, 25  
 IT 87-41-2, Phthalide 171-80-2, Spiro[cyclohexane-1,1'-phthalan]  
**496-14-0**, Phthalan 7111-66-2 35185-96-7,  
 1,4-Epoxy-1,2,3,4-tetrahydronaphthalene 42502-56-7, Isobenzofuran,  
 1,3-dihydro-1,1-dimethyl  
 (electron-transfer-induced reductive cleavage of phthalan  
 derivs.)

L50 ANSWER 8 OF 13 HCA COPYRIGHT 2002 ACS  
 124:55746 Reductive electrophilic substitution of phthalans and ring  
 expansion to isochroman derivatives. Azzena, Ugo; Demartis,  
 Salvatore; Fiori, Maria Giovanna; Melloni, Giovanni; Pisano, Luisa  
 (Dip. Chim., Univ. di Sassari, Sassari, I-07100, Italy).  
 Tetrahedron Letters, 36(44), 8123-6 (English) 1995. CODEN: TELEAY.  
 ISSN: 0040-4039. OTHER SOURCES: CASREACT 124:55746. Publisher:  
 Elsevier.

GI

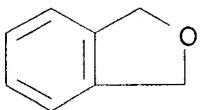


AB Reductive cleavage of phthalans I (R1 = H, R2 = H, Ph; R1R2 = CH2CH2) with Li and a catalytic amt. of naphthalene forms  
 stable arom. dilithium compds. II, which undergo ring  
 closure with CO2 to form isochromans III in yields >40%. II react  
 with various alkyl halides, aldehydes and ketones to form  
 o-substituted benzyl alcs. in yields > 60%.  
 IT **496-14-0**, Phthalan  
 (reductive electrophilic substitution of phthalans and ring  
 expansion to isochromanone derivs.)  
 RN 496-14-0 HCA  
 CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 27-14 (Heterocyclic Compounds (One Hetero Atom))  
 IT 100-52-7, Benzaldehyde, reactions 119-61-9, Benzophenone, reactions 496-14-0, Phthalan 630-19-3, 2,2-Dimethylpropionaldehyde 7111-66-2, Isobenzofuran, 1,3-dihydro,1-phenyl- 35185-96-7 (reductive electrophilic substitution of phthalans and ring expansion to isochromanone derivs.)

L50 ANSWER 9 OF 13 HCA COPYRIGHT 2002 ACS  
 117:25733 Cobalt-catalyzed oxidation of ethers using oxygen. Li, Pei; Alper, Howard (Ottawa-Carleton Chem. Inst., Univ. Ottawa, Ottawa, ON, K1N 6N5, Can.). J. Mol. Catal., 72(2), 143-52 (English) 1992. CODEN: JMCADS. ISSN: 0304-5102. OTHER SOURCES: CASREACT 117:25733.  
 AB Cobalt(II) chloride-catalyzed oxidn. of cyclic ethers with oxygen in 1,2-dimethoxyethane gives the corresponding lactones in reasonable to excellent yields. Oxidn. of acyclic alkyl benzyl ethers affords the corresponding esters in yields which are dependent on the stability of alkyl radicals. The more stable the alkyl radical, the lower the yield of the formed ester. Oxidn. of acyclic alkyl and heterocyclic ethers is also described. A radical mechanism is proposed involving participation of superoxocobalt.  
 IT 496-14-0 (autoxidn. of, mechanism of catalytic)  
 RN 496-14-0 HCA  
 CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 22-7 (Physical Organic Chemistry)  
 IT 103-50-4, Benzyl ether 109-99-9, reactions 142-96-1 493-05-0, Isochroman 496-14-0 538-86-3 539-30-0, Benzylethyl ether 946-80-5, Benzylphenyl ether 1612-65-3 1708-29-8, 2,5-Dihydrofuran (autoxidn. of, mechanism of catalytic)

L50 ANSWER 10 OF 13 HCA COPYRIGHT 2002 ACS  
 96:19300 Possible interactions of cyclobutadiene with by-products in inert matrix isolation studies. Fraga, Serafin (Dep. Chem., Univ. Alberta, Edmonton, AB, T6G 2G2, Can.). Tetrahedron Lett., 22(35), 3343-6 (English) 1981. CODEN: TELEAY. ISSN: 0040-4039.  
 AB A theor. study is reported of the complexes which may be formed by the in situ generation of cyclobutadiene with by-products in inert

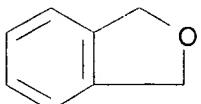
matrixes. **Stable** complexes are formed between cyclobutadiene and CO, HCN, phthalan, CO<sub>2</sub>, C<sub>6</sub>H<sub>6</sub>, and cyclobutadiene, though the **stabilization** energies are small (-8.4 to -2.0 kJ).

IT 496-14-0

(interaction of, with cyclobutadiene in inert matrixes, theor. calcn. of)

RN 496-14-0 HCA

CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 22-2 (Physical Organic Chemistry)

IT 71-43-2, reactions 74-90-8, properties 124-38-9, reactions

496-14-0 630-08-0, reactions

(interaction of, with cyclobutadiene in inert matrixes, theor. calcn. of)

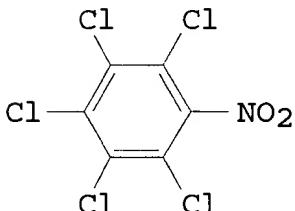
L50 ANSWER 11 OF 13 HCA COPYRIGHT 2002 ACS

90:49449 Study of the fungal resistance of plasticized **poly(vinyl chloride)**. Bochkareva, G. G.; Ovchinnikov,

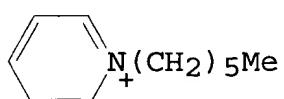
Yu. V.; Kurganova, L. N.; Beirekhova, V. A. (USSR).

Biopovrezhdeniya Mater. Zashch. Nikh, 151-3. Editor(s): Starostin, I. V. Izd. Nauka: Moscow, USSR. (Russian) 1978. CODEN: 39NJAS.

GI



I



Cl<sup>-</sup>

II

AB Penicillium funiculosum decompd. the protective dioctyl adipate [123-79-5] coating supplied as the only C source, forming fumaric acid [110-17-8]. The fungus also decompd. dioctyl sebacinate [2432-87-3], but not dioctyl phthalate [117-84-0] which was resistant even in the presence of sugar. The availability of sugar enhanced formation of enzymes by fungi and stimulated decompn. of PVC [9002-86-2] foils. The destruction of the protective coating by mold decreased the frost resistance of the foils. Only the foils contg. dioctyl phthalate retained their frost resistance after exposure to mold. Opaque clear PVC foils were protected from mold by captan [133-06-2], phthalan [

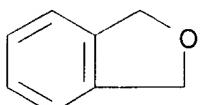
496-14-0], 0.5-1% pentachloronitrobenzene (I) [82-68-8], or 1-2% cetylpyridinium chloride (II) [123-03-5], while transparent foils were protected by 0.1-0.3% bis(tributyltin oxide) [56-35-9] or tributyltin acetate [56-36-0].

IT 496-14-0

(mold control by, on PVC)

RN 496-14-0 HCA

CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



IT 9002-86-2

(mold control on)

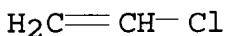
RN 9002-86-2 HCA

CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4

CMF C2 H3 Cl



CC 5-2 (Agrochemicals)

ST PVC protective coating mold fungicide

IT Penicillium funiculosum

(PVC coatings response to)

IT Mold (fungus)

(control of, on PVC)

IT Fungicides and Fungistats

(for PVC)

IT 117-84-0 123-79-5 2432-87-3

(catabolism of, by mold, PVC degrdn. in relation to)

IT 56-35-9 56-36-0 82-68-8 123-03-5 133-06-2 496-14-0

(mold control by, on PVC)

IT 9002-86-2

(mold control on)

L50 ANSWER 12 OF 13 HCA COPYRIGHT 2002 ACS

89:195587 Effect of storage on pesticide residues in canned food.

Timofeeva, O. A.; Shvartsman, G. A.; Pyshnaya, E. G. (Mold.

Nauchno-Issled. Inst. Pishchevoi Prom., Kishinev, USSR). Konservn.

Ovoshchesush. Prom-st. (9), 10-12 (Russian) 1978. CODEN: KOPRAU.

ISSN: 0023-3587.

AB Hexachlorobutadiene [87-68-3] was very **stable** in canned grape juice during storage for 2 yr. In open cans it disappeared in a few days.  $\gamma$ -Hexachlorocyclohexane [58-89-9] decreased only

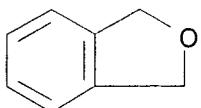
slightly in canned plum compote during 2 yr of storage. Phthalan [496-14-0] decreased to zero in canned grape juice during 4 yr of storage. Carbophos [121-75-5] decreased very slowly in both canned products, whereas Anthio [2540-82-1] decreased rapidly; however, the latter formed the toxic compd. phosphamide [60-51-5], which was **stable**. Therefore, storage of canned juices or compotes is not a dependable method of reducing their fungicide and insecticide residues.

IT 496-14-0

(of canned fruits and juice, storage effect on)

RN 496-14-0 HCA

CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 17-2 (Foods)

Section cross-reference(s): 5

IT 58-89-9 60-51-5 87-68-3 121-75-5 496-14-0

2540-82-1

(of canned fruits and juice, storage effect on)

L50 ANSWER 13 OF 13 HCA COPYRIGHT 2002 ACS

68:28708 Activity of some fungicides on tomato Phytophthora. Granin, E. F.; Izubenko, V. V. Khim. Sel'sk. Khoz., 5(5), 347-51 (Russian) 1967. CODEN: KSKZAN.

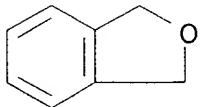
AB Tomato plants 15-18 cm. tall were sprayed with fungicide suspensions (9 .mu.L/cm<sup>2</sup>) and infected with P. infestans. The most effective fungicides were marzine (total protection by a 0.04% suspension), zineb, figone, captan, and polycarbazine. Kuprazine 1, phthalan, ferbam, and ziram were less effective, while CuCl<sub>2</sub>, even when used in high concns. (0.5%), did not give total protection. The loss of activity caused by direct sunlight and moisture was high for marzine, but was smaller for polycarbazine; CuCl<sub>2</sub> was the most **stable** fungicide tested. 14 references.

IT 496-14-0

(Phytophthora infestans control by, on tomatoes)

RN 496-14-0 HCA

CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 19 (Pesticides)

IT 117-80-6 133-06-2 137-30-4 303-25-3 496-14-0

7447-39-4 8065-68-7 9006-42-2 12122-67-7 12427-38-2

14484-64-1

(Phytophthora infestans control by, on tomatoes)

=&gt; d 151 1-7 cbib abs hitstr hitind

L51 ANSWER 1 OF 7 HCA COPYRIGHT 2002 ACS

136:247398 Etherification method for producing benzyl ether derivatives of 2-butene-1,4-diols. Krishnamurti, Ramesh; Wang, Qi; Smolka, Thomas F. (Occidental Chemical Corporation, USA; Stephens, Dinah, H.). PCT Int. Appl. WO 2002022537 A2 20020321, 19 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-GB4036 20010910. PRIORITY: US 2000-PV231790 20000911.

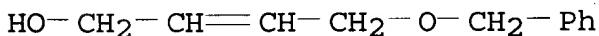
AB A method for producing benzyl ethers of 2-butene-1,4-diols, useful as polymer **stabilizers** (no data), comprises reacting 2-butene-1,4-diols (e.g., 2-butene-1,4-diol) with benzyl chlorides (e.g., benzyl chloride) in the presence of an alkali (e.g., sodium hydroxide) or alk. earth metal hydroxide or carbonate, optionally in the presence of a phase-transfer catalyst (e.g., benzyltriethylammonium chloride) to produce mono- and/or di-benzyl ethers of 2-butene-1,4-diols [e.g., 1,4-bis(benzylloxy)-2-butene] and recovering at least a portion of at least one such benzene deriv.

IT 80885-30-9P

(etherification method for producing benzyl ether derivs. of 2-butene-1,4-diols)

RN 80885-30-9 HCA

CN 2-Buten-1-ol, 4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



IC ICM C07C041-00

CC 25-9 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 37, 45

IT 70677-94-0P, 1,4-Bis(benzylloxy)-2-butene 80885-30-9P

(etherification method for producing benzyl ether derivs. of 2-butene-1,4-diols)

L51 ANSWER 2 OF 7 HCA COPYRIGHT 2002 ACS

136:102461 **Stability**, Reactivity, Solution, and Solid-State Structure of Halomethylzinc Alkoxides. Charette, Andre B.; Molinaro, Carmela; Brochu, Christian (Departement de Chimie, Universite de Montreal, Montreal, QC, H3C 3J7, Can.). Journal of the American Chemical Society, 123(49), 12160-12167 (English) 2001.

CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB The development of a Lewis acid-catalyzed cyclopropanation of allylic alcs. with bis(iodomethyl)zinc is reported. Iodomethylzinc alkoxides (e.g., chloro- and iodomethyl zinc 4-methoxybenzyloxy compds.) can be formed by treatment of an alc. with bis(iodomethyl)zinc, and their crystal structures solved. These species are not prone to undergo cyclopropanation at low temp., but the addn. of a Lewis acid in catalytic amts. induces the cyclopropanation reaction. Thus, CH<sub>2</sub>I<sub>2</sub> and Et<sub>2</sub>Zn were stirred and added to cinnamyl alc. in the presence of TiC<sub>4</sub>, to give the cyclopropanation product, trans-(3-phenylcyclopropyl)methanol, in ~90% yield. The Lewis acid-catalyzed pathway significantly overwhelms the uncatalyzed one. The prepn. and **stability** of halomethyl zinc alkoxides in soln., their aggregation state in soln., and solid-state structures are discussed. Furthermore, the competition reaction between the inter- vs. intramol. cyclopropanation is studied. Finally, the possible activation pathways to explain the Lewis acid activation of halomethylzinc alkoxides is discussed.

IT 81028-03-7

(Lewis acid-catalyzed cyclopropanation of allylic alcs. with bis(halomethyl)zinc)

RN 81028-03-7 HCA

CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



CC 29-9 (Organometallic and Organometalloidal Compounds)  
Section cross-reference(s): 22, 75

IT Metal alkoxides

(**stability**, reactivity, soln., and solid-state structure of halomethylzinc alkoxides)

IT 60-12-8, Phenethyl alcohol 67-64-1, Acetone, reactions 75-11-6,  
Diodomethane 100-44-7, Benzyl chloride, reactions 105-13-5,  
4-Methoxybenzyl alcohol 122-97-4, 3-Phenyl-1-propanol 556-82-1  
557-20-0, Diethyl zinc 928-95-0 1576-95-0 4845-04-9,  
1-Cyclohexene-1-methanol 36004-04-3 55131-20-9 75553-23-0  
81028-03-7 87770-83-0 388568-84-1

(Lewis acid-catalyzed cyclopropanation of allylic alcs. with bis(halomethyl)zinc)

L51 ANSWER 3 OF 7 HCA COPYRIGHT 2002 ACS

135:272544 One-pot oxidation and wittig olefination of alcohols using o-iodoxybenzoic acid and **stable** wittig ylide. Maiti, Arup; Yadav, J. S. (Organic Division, Indian Institute of Chemical Technology, Hyderabad, 500007, India). Synthetic Communications, 31(10), 1499-1506 (English) 2001. CODEN: SYNCAV. ISSN: 0039-7911.

Publisher: Marcel Dekker, Inc..

AB Benzylic, allylic, and propargylic alcs., as well as diols, can be oxidized with o-iodoxybenzoic acid (IBX) in the presence of **stabilized** Wittig ylide to generate .alpha.,.beta.-unsatd. ester in one pot. This is useful when the intermediate aldehydes are unstable and difficult to isolate. For example, to a soln. of benzenemethanol in dimethylsulfoxide was added a mixt. of (triphenylphosphoranylidene)acid Et ester and 2-iodoxybenzoic acid. The yield of Et cinnamate thus prep'd. was 98%.

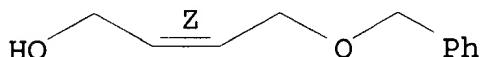
IT 81028-03-7

(prepn. of .alpha.,.beta.-unsatd. esters by one-pot oxidn. and Wittig olefination of alcs. using iodoxybenzoic acid and (triphenylphosphoranylidene)acetate (Wittig ylide))

RN 81028-03-7 HCA

CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



CC 21-2 (General Organic Chemistry)

IT 100-51-6, Benzenemethanol, reactions 106-24-1 107-19-7,  
2-Propyn-1-ol 107-21-1, 1,2-Ethanediol, reactions 504-63-2,  
1,3-Propanediol 821-11-4 1099-45-2,  
(Triphenylphosphoranylidene)acetic acid ethyl ester 4407-36-7  
4541-14-4 20739-58-6, 2-Octyn-1-ol 64297-64-9, 2-Iodoxybenzoic  
acid 81028-03-7

(prepn. of .alpha.,.beta.-unsatd. esters by one-pot oxidn. and Wittig olefination of alcs. using iodoxybenzoic acid and (triphenylphosphoranylidene)acetate (Wittig ylide))

L51 ANSWER 4 OF 7 HCA COPYRIGHT 2002 ACS

135:93426 **Stabilization** of polymers after exposure to oxidation and article manufacture. Wang, Qi (USA). U.S. Pat. Appl. Publ. US 20010007884 A1 20010712, 9 pp., Cont.-in-part of U. S. Ser. No. 272,843. (English). CODEN: USXXCO. APPLICATION: US 2001-761625 20010117. PRIORITY: US 1999-272843 19990319.

AB **Polyvinyl chloride**, **polyvinylidene chloride**, **polycarbonate**, **polyethylene**, **polypropylene**, polyamide, polyimide, polyether, polyester, or polyvinyl acetate contg. .apprx.0.005-10 phr **stabilizer** are resistant to discoloring after exposure to oxidn. PVC contg. 1.34 g **stabilizer** phthalan had initial yellowness value 17.5, after .gamma. radiation 31.9, and after aging 49.5, vs. 18.1, 50.2, and 75.5, resp., for a control without **stabilizer**.

IT 81028-03-7

(**stabilization** of polymers after exposure to oxidn.)

RN 81028-03-7 HCA

CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

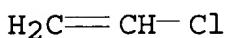


IT 9002-86-2, Poly(vinyl chloride)  
 ) 9002-88-4, Polyethylene 9003-07-0,  
**Polypropylene**  
 (stabilization of polymers after exposure to oxidn.)

RN 9002-86-2 HCA  
 CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

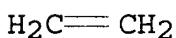
CRN 75-01-4  
 CMF C<sub>2</sub> H<sub>3</sub> Cl



RN 9002-88-4 HCA  
 CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

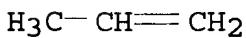
CRN 74-85-1  
 CMF C<sub>2</sub> H<sub>4</sub>



RN 9003-07-0 HCA  
 CN 1-Propene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 115-07-1  
 CMF C<sub>3</sub> H<sub>6</sub>



IC ICM C08K005-06  
 ICS C08K005-46

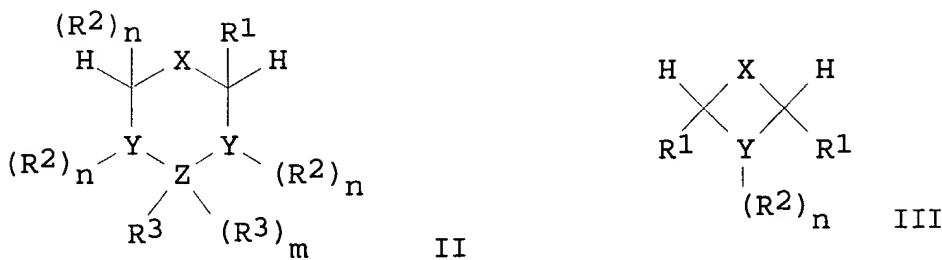
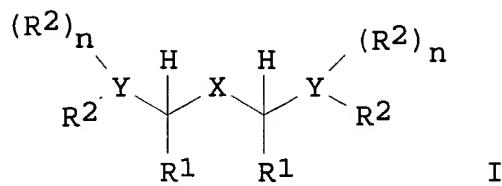
NCL 524083000

CC 37-6 (Plastics Manufacture and Processing)  
 ST discoloration prevention agents polymer; PVC phthalan  
 stabilizer; polyvinylidene chloride yellowing prevention;  
 polycarbonate yellowing prevention; polyethylene  
 yellowing prevention; polypropylene yellowing prevention;

polyamide yellowing prevention; polyimide yellowing prevention;  
 polyether yellowing prevention; polyester yellowing prevention;  
 polyvinyl acetate yellowing prevention  
 IT Antioxidants  
 Discoloration prevention agents  
 Yellowing prevention  
 (stabilization of polymers after exposure to oxidn.)  
 IT Polyamides, uses  
 Polycarbonates, uses  
 Polyesters, uses  
 Polyethers, uses  
 Polyimides, uses  
 Polyurethanes, uses  
 (stabilization of polymers after exposure to oxidn.)  
 IT 110-65-6, 2-Butyne-1,4-diol 332-77-4 496-14-0, Phthalan  
 589-29-7, 1,4-Benzenedimethanol 1606-85-5, 1,4-Bis(2-hydroxy  
 ethoxy)-2-butyne 2568-24-3 5417-32-3 10192-64-0 21285-46-1  
 67461-24-9 68972-96-3 **81028-03-7**  
 (stabilization of polymers after exposure to oxidn.)  
 IT 9002-85-1, Poly(vinylidene chloride) **9002-86-2**,  
 Poly(vinyl chloride) **9002-88-4**  
 , Polyethylene **9003-07-0**, Polypropylene  
 9003-20-7, Poly(vinyl acetate)  
 (stabilization of polymers after exposure to oxidn.)

L51 ANSWER 5 OF 7 HCA COPYRIGHT 2002 ACS  
 133:267624 **Stabilization** and discoloration prevention of  
 polymers after exposure to oxidation and antioxidants therefor.  
 Wang, Qi (Occidental Chemical Corporation, USA; Stephens, Dinah).  
 PCT Int. Appl. WO 2000056812 A1 20000928, 37 pp. DESIGNATED STATES:  
 W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,  
 CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN,  
 IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG,  
 MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,  
 TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD,  
 RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES,  
 FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD,  
 TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-GB247  
 20000128. PRIORITY: US 1999-272843 19990319.

GI



AB **Poly(vinyl chloride), poly(vinylidene chloride), polycarbonates, polyethylene, polypropylene, polyamides, polyimides, polyethers, polyesters, or poly(vinyl acetate) contg. apprx.0.005-10 phr of a stabilizer I, II, or III, where Z is C, P, Sn, Si, or B; X is -R1C:CR1-, ethynyl, (un)substituted benzene, pyridine, pyrimidine, triazine, furan, pyrrole, thiophene, or naphthalene ring; each Y is independently O, S, or N; each R is independently H, C1-24-alkyl, C6-24-aryl, C7-24-aralkyl; each R1 is independently R, OR, RCO, ROCO, ROCO2, PR2, P(OR)2, PR(OR), NR2, R2NCO, R2NCO2, SR, halogen, or two R1 groups can form a ring; each R2 is independently R, RCO, ROCO, P(OR)2, Sn(R)q(OR)3-q, SnRq(OCOR)3-q, Si(R)q(OR)3-q, BRq(OR)2-q, or two R2 groups can form a ring; each R3 is independently R, RCO, ROCO, ROCO2, OR, SR, NR2, OPR2, or OP(OR)2; m is 0 when Z is P or B and 1 when Z is Sn, Si, or C; n is 0 when Y is O or S and 1 when Y is N; p is 0-4; and q is 0-3 for the tin stabilizers and 0-2 for the boron stabilizers, with the proviso that in I, when X = -CH:CH-, Y = O and R2 = H, at least one of the R1 is not H; and in II, when X = -R1C:CR1-, Y = O and Z = C, then at least one of the R3 groups on Z is not H. Thus, a plaque from a compn. comprising PVC 150.00, stearic acid 0.30, Mark 152S 0.23, dioctyl phthalate 97.50, Drapex 6.8 15.00, and phthalan 1.34 g was irradiated with 50 kGy .gamma.-rays, and aged 48 h at 50.degree., giving yellowness 17.5 initially, 31.9 after radiation, and 49.5 after aging, compared with 18.1, 50.2, and 75.5, resp., without phthalan.**

IT 81028-03-7, cis-4-Benzylxy-2-buten-1-ol  
(stabilization and discoloration prevention of polymers  
after exposure to oxidn. and antioxidants therefor)

RN 81028-03-7 HCA  
CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT 9002-86-2, PVC 9002-88-4,  
**Polyethylene 9003-07-0, Polypropylene**  
 (stabilization and discoloration prevention of polymers  
 after exposure to oxidn. and antioxidants therefor)

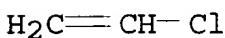
RN 9002-86-2 HCA

CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4

CMF C2 H3 Cl



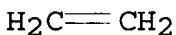
RN 9002-88-4 HCA

CN Ethene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 74-85-1

CMF C2 H4



RN 9003-07-0 HCA

CN 1-Propene, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 115-07-1

CMF C3 H6



IC ICM C08K005-00

ICS C08K005-053; C08K005-15; C08K005-06

CC 37-6 (Plastics Manufacture and Processing)

ST antioxidant yellowing prevention polymer; PVC phthalan  
 antioxidant gamma radiation; polyolefin antioxidant yellowing  
 prevention; vinyl compd polymer antioxidant yellowing prevention;  
**polycarbonate antioxidant yellowing prevention;**  
**polyurethane antioxidant yellowing prevention;** polyamide

antioxidant yellowing prevention; polyimide antioxidant yellowing prevention; polyether antioxidant yellowing prevention; polyester antioxidant yellowing prevention

IT Yellowing prevention  
 Yellowing prevention  
 (agents; **stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT Antioxidants  
 (**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT Polyamides, uses  
**Polycarbonates**, uses  
 Polyesters, uses  
 Polyethers, uses  
 Polyimides, uses  
**Polyurethanes**, uses  
 (**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT Discoloration prevention agents  
 Discoloration prevention agents  
 (yellowing; **stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT 110-64-5, 2-Butene-1,4-diol 110-65-6, 2-Butyne-1,4-diol  
 332-77-4, 2,5-Dimethoxy-2,5-dihydrofuran 496-14-0, Phthalan  
 589-29-7, 1,4-Benzenedimethanol 1606-85-5, 1,4-Bis(2-hydroxyethoxy)-2-butyne 2568-24-3, 4,7-Dihydro-2-phenyl-1,3-dioxepin 10192-64-0 21285-46-1 67461-24-9 68972-96-3, cis-1,4-Bisbenzyloxy-2-butene 70677-94-0 81028-03-7, cis-4-Benzylbenzoate  
 (**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

IT 9002-85-1, Poly(vinylidene chloride) 9002-86-2,  
 PVC 9002-88-4, **Polyethylene**  
 9003-07-0, **Polypropylene** 9003-20-7, Poly(vinyl acetate)  
 (**stabilization** and discoloration prevention of polymers after exposure to oxidn. and antioxidants therefor)

L51 ANSWER 6 OF 7 HCA COPYRIGHT 2002 ACS

131:257029 Deprotection of tetrahydropyranyl ethers with montmorillonite K-10 clay in methanol. Taniguchi, Takahiko; Kadota, Kohei; ElAzab, Adel S.; Ogasawara, Kunio (Pharmaceutical Institute, Tohoku Univ., Sendai, 980, Japan). *Synlett* (8), 1247-1248 (English) 1999. CODEN: SYNLES. ISSN: 0936-5214. OTHER SOURCES: CASREACT 131:257029.

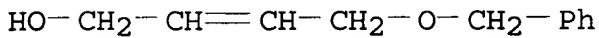
Publisher: Georg Thieme Verlag.

AB A variety of tetrahydropyranyl (THP) ethers are cleaved by montmorillonite K-10 clay in MeOH at room temp. to give the corresponding alcs. THP ethers carrying epoxy, MeOCH<sub>2</sub>O, Me<sub>3</sub>CPh<sub>2</sub>SiO, ACO, and PhCO<sub>2</sub> functionalities are **stable** under the conditions, while ethers carrying ketal, Me<sub>3</sub>CMe<sub>2</sub>SiO, and Cl<sub>3</sub>CC(:NH)O functionalities are unstable.

IT 80885-30-9P

(deprotection of hydroxyl ethers with montmorillonite K-10 in methanol)

RN 80885-30-9 HCA  
 CN 2-Buten-1-ol, 4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



CC 21-2 (General Organic Chemistry)

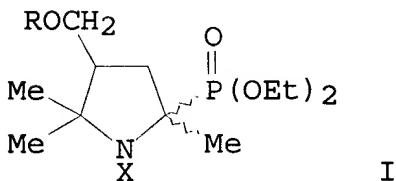
IT 57-88-5P, Cholest-5-en-3-ol (3. $\beta$ .)-, preparation 89-78-1P  
 98-00-0P, 2-Furanmethanol 100-02-7P, 4-Nitrophenol, preparation  
 100-51-6P, Benzyl alcohol, preparation 108-95-2P, Phenol,  
 preparation 111-70-6P, 1-Heptanol 150-76-5P, 4-Methoxyphenol  
 768-95-6P, Tricyclo[3.3.1.13,7]decan-1-ol 1471-15-4P 4541-14-4P  
 6318-30-5P 13482-22-9P 32651-37-9P 35435-68-8P 51326-51-3P  
**80885-30-9P** 87184-99-4P 95672-91-6P 101992-89-6P  
 130372-07-5P 244298-24-6P 244298-25-7P 244298-46-2P  
 244298-47-3P 244781-68-8P

(deprotection of hydroxyl ethers with montmorillonite K-10 in methanol)

L51 ANSWER 7 OF 7 HCA COPYRIGHT 2002 ACS

119:117385  $\beta$ -Phosphorylated five-membered ring nitroxides:  
 synthesis and ESR study of 2-phosphonyl-4-(hydroxymethyl)pyrrolidine  
 aminoxy radical. Stipa, Pierluigi; Finet, Jean Pierre; Le Moigne,  
 Francois; Tordo, Paul (Lab. Struct. React. Espèces Paramagn., Univ.  
 Provence, Marseille, 13397, Fr.). J. Org. Chem., 58(16), 4465-8  
 (English) 1993. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES:  
 CASREACT 119:117385.

GI



AB Intramol. aminomercuration of the alkenyl  $\alpha$ -amino phosphonate  $\text{PhCH}_2\text{OCH}_2\text{CH}(\text{CMe}:\text{CH}_2)\text{CH}_2\text{CMe}(\text{NH}_2)\text{P}(\text{O})(\text{OEt})_2$  followed by sodium borohydride redn. leads to the di-Et [4-(benzyloxymethyl)-2,5,5-trimethylpyrrolidinyl]phosphonate I (R = PhCH<sub>2</sub>, X = H). Oxidn. of the phosphonates I (R = H, PhCH<sub>2</sub>; X = H) with 3-chloroperbenzoic acid led to the **stable** 2-phosphonylpolyrrolidinyl aminoxy radicals I (same R; X = O.bul.) bearing a 4-(hydroxymethyl) substituent.

IT 81028-03-7

(oxidn. of)  
 RN 81028-03-7 HCA  
 CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



CC 29-7 (Organometallic and Organometalloidal Compounds)  
 Section cross-reference(s): 22  
 IT 81028-03-7  
 (oxidn. of)

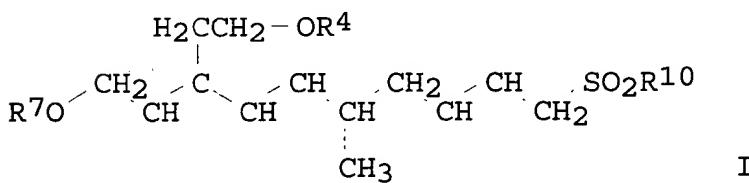
=> d his 161-

FILE 'LCA' ENTERED AT 17:48:28 ON 28 AUG 2002  
 L61 14809 S (INHIBIT? OR HINDER? OR IMPED? OR ARREST? OR REDUC? OR  
 L62 623 S ANTIOXID? OR (ANTI OR INHIBIT? OR HINDER? OR IMPED? OR  
 FILE 'HCA' ENTERED AT 17:49:47 ON 28 AUG 2002  
 L63 8 S (L30 OR L31 OR L32) AND L62  
 L64 5 S L63 NOT (L49 OR L50 OR L51)

=> d 164 1-5 cbib abs hitstr hitind

L64 ANSWER 1 OF 5 HCA COPYRIGHT 2002 ACS  
 136:294537 Preparation of bongrekic acid precursors. Shishido, Kozo;  
 Shindo, Mitsuru; Shinohara, Yasuo; Terada, Hiroshi (Foundation for  
 Scientific Technology Promotion, Japan). Jpn. Kokai Tokkyo Koho JP  
 2002105045 A2 20020410, 35 pp. (Japanese). CODEN: JKXXAF.  
 APPLICATION: JP 2001-6736 20010115. PRIORITY: JP 2000-224369  
 20000725.

GI



AB C1-10 segment of bongrekic acid I (R6, R7 = tert-  
 butyldiphenylsilyl, triisopropylsilyl, tert-butyldimethylsilyl,

triethylsilyl; R10 = lower alkyl, aryl) are prep'd. by reaction of R1COCH<sub>2</sub>Me (R1 = substituted 2-oxo-1,3-oxazolidin-3-yl, camphorsultam ring) with X<sub>1</sub>CH<sub>2</sub>CH:CHCH<sub>2</sub>OR<sub>5</sub> (R<sub>5</sub> = corresponding to R<sub>6</sub>; X<sub>1</sub> = halo), **redn.**, **oxidn.**, condensation with R<sub>8</sub>OB(OR<sub>9</sub>)CHCl<sub>2</sub>

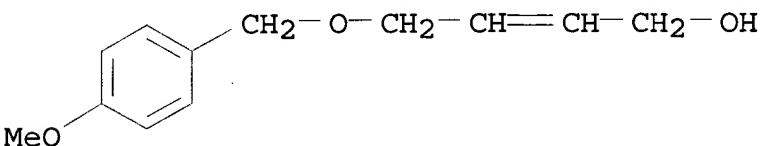
(R<sub>8</sub>, R<sub>9</sub> = alkyl, R<sub>8</sub>R<sub>9</sub> may form alkylene), coupling reaction with HOCH<sub>2</sub>CH:CICH<sub>2</sub>CH<sub>2</sub>OR<sub>6</sub> (R<sub>6</sub> = same as I), reaction with R<sub>7</sub>X<sub>2</sub> (R<sub>7</sub> = same as I; X<sub>2</sub> = halo), deprotection, halogenation, and reaction with R<sub>10</sub>SO<sub>2</sub>M (R<sub>10</sub> = lower alkyl, aryl; M = alkali metal). C<sub>11</sub>-22 segment of bongrekic acid is also manufd. from furanones in eight steps. (2Z,4E,6S,8E)-10-chloro-3-[2-(4-methoxybenzyloxy)ethyl]-1-(methoxymethoxy)-6-methyl-2,4,8-decatriene (prepn. given) was reacted with PhSO<sub>2</sub>Na in DMF at room temp. for 20.5 h to give 87% (2Z,4E,6S,8E)-10-phenylsulfonyl-3-[2-(4-methoxybenzyloxy)ethyl]-1-(methoxymethoxy)-6-methyl-2,4,8-decatriene.

IT 409064-73-9P

(prepn. of bongrekic acid precursors)

RN 409064-73-9 HCA

CN 2-Buten-1-ol, 4-[(4-methoxyphenyl)methoxy]- (9CI) (CA INDEX NAME)



IC ICM C07C315-04

ICS C07C317-18; C07C317-22

CC 23-12 (Aliphatic Compounds)

IT 1707-77-3P, 1,2:5,6-Di-O-isopropylidene-D-mannitol 2060-25-5P,

3-Bromo-2-propyn-1-ol 37428-55-0P 76236-32-3P 78508-96-0P,

(S)-5-Hydroxy-2-penten-4-oxide 81480-31-1P, (S)-4-Methyl-5-trityloxymethyl-2(5H)-furanone 81677-37-4P, (E)-5-tert-

Butyldiphenylsilyloxy-3-penten-1-yne 112837-18-0P,

(S)-5-Hydroxymethyl-4-methyl-2(5H)-furanone 142860-83-1P

145222-40-8P, 4-(4-Methoxybenzyloxy)-2-butyn-1-ol 146916-76-9P

152126-99-3P, 4-tert-Butyldiphenylsilyloxy-2-buten-1-ol

210056-70-5P, 1-tert-Butyldiphenylsilyloxy-4-iodo-2-butene

397333-59-4P, (E)-1-Bromo-3-tert-butyldiphenylsilyloxy-1-propene

409064-73-9P 409064-74-0P, 1-tert-Butyldiphenylsilyloxy-4-

(4-methoxybenzyloxy)-2-butene 409064-75-1P, 1-Bromo-4-tert-

butyldiphenylsilyloxy-2-butene 409064-76-2P, (Z)-3-Iodo-5-(4-

methoxybenzyloxy)-2-penten-1-ol 409064-87-5P 409064-88-6P

409064-89-7P 409064-90-0P 409064-97-7P, Ethyl

(2E,4Z,6R,10E)-12-tert-butyldiphenylsilyloxy-6-hydroxy-2,5-dimethyl-

2,4,10-dodecatriene-8-ynoate 409064-98-8P, Ethyl

(2E,4Z,6R,10E)-12-tert-butyldiphenylsilyloxy-6-methoxy-2,5-dimethyl-

2,4,10-dodecatriene-8-ynoate 409064-99-9P, Ethyl

(2E,4Z,6R,8Z,10E)-12-tert-butyldiphenylsilyloxy-6-methoxy-2,5-

dimethyl-2,4,8,10-dodecatetraenoate

(prepn. of bongrekic acid precursors)

L64 ANSWER 2 OF 5 HCA COPYRIGHT 2002 ACS

130:227519 Skin care cosmetics containing humectants and rough skin-improving agents. Nanba, Tomiyuki; Kaminuma, Mikiko; Okamoto, Akira; Nakajima, Hideo (Shiseido Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 11035443 A2 19990209 Heisei, 14 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1997-207150 19970716.

AB Skin care cosmetics contg. lower alkyl tetritol ethers as humectants and rough skin-improving agents are claimed. A cosmetic lotion contain propylene glycol 5.0, citric acid 4.0, monomethyl erythritol ether 3.0, 95% ethanol 8.0, POE lauryl ether 2.0, **antioxidants** and preservatives, perfumes and ion-exchanged water to 100%.

IT 81028-03-7P  
(skin care cosmetics contg. humectants and rough skin-improving agents)

RN 81028-03-7 HCA

CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IC ICM A61K007-48

ICS A61K007-00; A61K009-06

CC 62-4 (Essential Oils and Cosmetics)

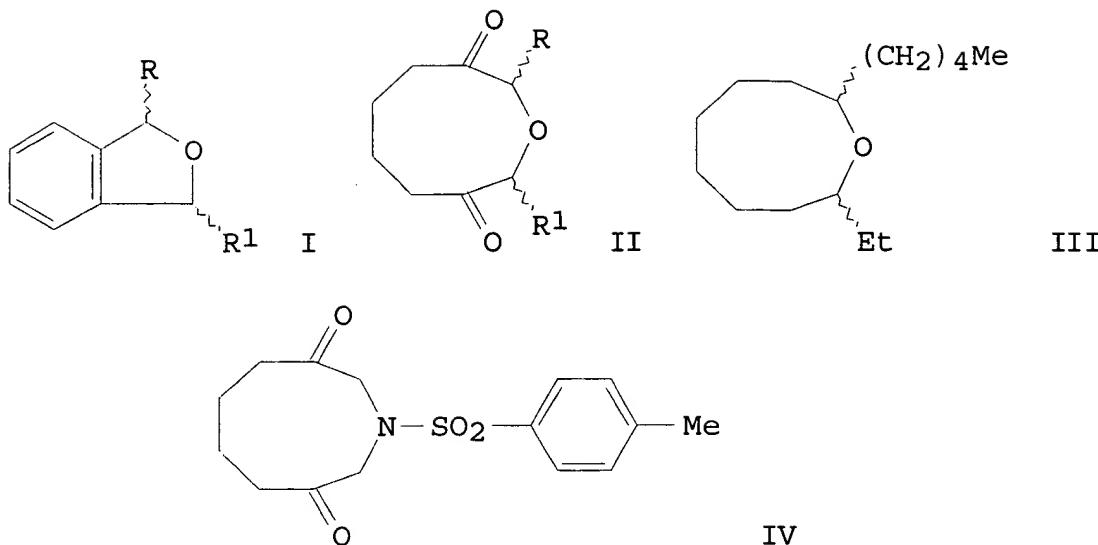
IT 81028-03-7P 85514-70-1P 99903-84-1P 122887-79-0P  
221000-57-3P 221000-58-4P 221000-59-5P 221000-60-8P  
(skin care cosmetics contg. humectants and rough skin-improving agents)

L64 ANSWER 3 OF 5 HCA COPYRIGHT 2002 ACS

120:323072 Preparation of 9-membered cyclic ethers from phthalans.

Synthesis of obtusan. Elliott, Mark C.; Moody, Christopher J. (Dep. Chem., Loughborough Univ. Technol., Loughborough/Leicestershire, LE11 3TU, UK). Synlett (12), 909-10 (English) 1993. CODEN: SYNLES. ISSN: 0936-5214. OTHER SOURCES: CASREACT 120:323072.

GI

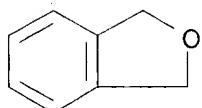


AB Phthalans I [R = R1 = H; R = Et, (CH<sub>2</sub>)<sub>4</sub>Me, R1 = H; R = (CH<sub>2</sub>)<sub>4</sub>Me, R1 = Et] have been converted into oxonane-3,8-diones II by a 3-step sequence involving Birch **redn.**, hydrogenation and **oxidative** cleavage; the 2-ethyl-9-pentyl deriv. II [R = (CH<sub>2</sub>)<sub>4</sub>Me, R1 = Et] has been deoxygenated to give obtusan III. The method was extended to the prepn. of azonane IV from isoindoline.

IT 496-14-0, Phthalan  
(reactant, in prepn. of nine-membered cyclic ethers from  
phthalans and synthesis of obtusan)

RN 496-14-0 HCA

CN Isobenzofuran, 1,3-dihydro- (9CI) (CA INDEX NAME)



CC 26-9 (Biomolecules and Their Synthetic Analogs)

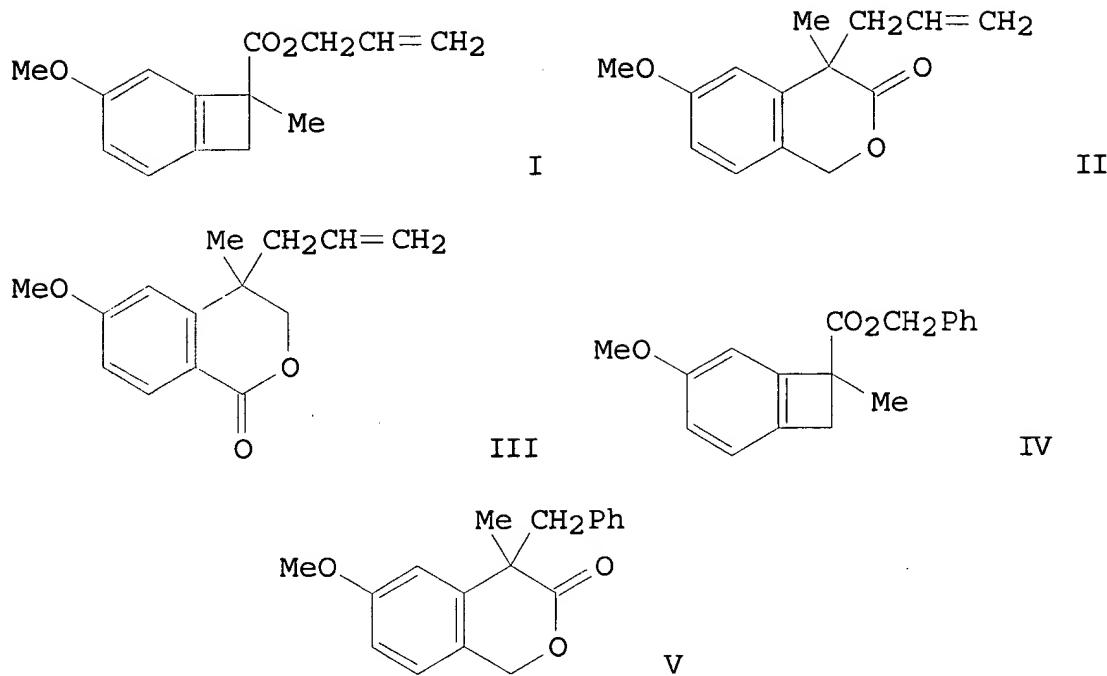
IT 496-12-8, Isoindoline 496-14-0, Phthalan 628-17-1,  
Pentyl iodide

(reactant, in prepn. of nine-membered cyclic ethers from phthalans and synthesis of obtusan)

L64 ANSWER 4 OF 5 HCA COPYRIGHT 2002 ACS

103:215122 Tandem electrocyclic-sigmatropic reaction of benzocyclobutenes. An expedient route to 4,4-disubstituted isochromanones. Shishido, Kozo; Shitara, Eiki; Fukumoto, Keiichiro; Kametani, Tetsuji (Pharm. Inst., Tohoku Univ., Sendai, 980, Japan). J. Am. Chem. Soc., 107(20), 5810-12 (English) 1985. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT 103:215122.

GI



AB A novel and useful tandem electrocyclic-sigmatropic reaction of benzocyclobutenes was described. The thermolysis of 1-alkyl-1-carballyloxybenzocyclobutenes e.g. I, readily derivable from 1-cyanobenzocyclobutene, gave 4-alkyl-4-allyl-isochroman-3-ones, e.g. III, via a tandem electrocyclic-[3,3]sigmatropic reaction in excellent yields. II was converted quant. to the isochroman-1-one III by a two-step **redn.-oxidn.** sequence. Thermolysis of 1-alkyl-1-carbobenzyloxybenzocyclobutenes e.g. IV gave 4-alkyl-4-benzylisochroman-3-ones, e.g. V, via a tandem electrocyclic-[1,3]sigmatropic reaction. Those results provide a general and efficient procedure for constructing the isochromanones with quaternary carbon on a benzylic carbon. The isochromanones are synthons for Amaryllidaceae alkaloids.

IT 69152-88-1 81028-03-7

(esterification by, of benzocyclobutene carboxylic acid deriv.)

RN 69152-88-1 HCA

CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 81028-03-7 HCA  
 CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

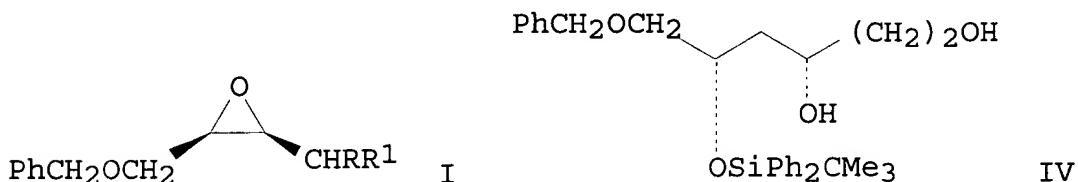


CC 27-14 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 31  
 IT 100-51-6, reactions 105-13-5 107-19-7 586-98-1 636-72-6  
 2028-63-9 21964-44-3 51410-44-7 69152-88-1  
**81028-03-7**  
 (esterification by, of benzocyclobutene carboxylic acid deriv.)

L64 ANSWER 5 OF 5 HCA COPYRIGHT 2002 ACS

98:88772 Stereocontrolled synthesis of 1,3,5... (2n + 1) polyols.  
 Nicolaou, K. C.; Uenishi, J. (Dep. Chem., Univ. Pennsylvania,  
 Philadelphia, PA, 19104, USA). J. Chem. Soc., Chem. Commun. (22),  
 1292-3 (English) 1982. CODEN: JCCCAT. ISSN: 0022-4936.

GI

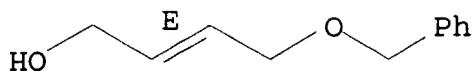


AB The stereoselective prepn. of 1,3,5... (2n + 1)-polyols based on the Sharpless asym. epoxidn. and regioselective ring opening by (Me2CHCH2)2AlH is reported. E.g., epoxidn. of (E)-PhCH2OCH2CH:CHCH2OH with Me3COOH in CH2Cl2 contg. Ti(OCHMe2)4 and di-Et (-)-tartrate at -23.degree. gave 80% epoxide I (R = H, R1 = OH) which on oxidn. and Wittig reaction with Ph3P:CHCO2Me gave I (RR1 = CHCO2Me) (II) as a 84:16 E:Z mixt. Ring opening of II with (Me2CHCH2)2AlH in CH2Cl2 at -78.degree. and protection of the hydroxyl group gave PhCH2OCH2CH(OSiPh2CMe3)CH2CH:CHCH2OH (III). Epoxidn. of III as above followed by redn. with NaAl2(OCH2CH2OMe)2 in THF at 0-25.degree. gave alc. IV.

IT 69152-88-1  
 (epoxidn. of, stereospecific)

RN 69152-88-1 HCA  
 CN 2-Buten-1-ol, 4-(phenylmethoxy)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



CC 23-7 (Aliphatic Compounds)

Section cross-reference(s): 27, 33

IT 69152-88-1

(epoxidn. of, stereospecific)

IT 84582-67-2P

(prepn., epoxidn., redn., oxidn., and Wittig reactions of)